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On the Coincidence of M_1-Maximal and $\widetilde{M}_2$-Maximal Graphs

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Abstract

Let G be a simple graph with degree sequence $(d_1, d_2, \ldots, d_n)$. The first and second Zagreb indices are defined respectively as the quantities $M_1(G) = \sum_{i=1}^{n} d_i^2$ and $M_2(G) = \sum_{v_i v_j \in E(G)} d_i d_j$. The Nordhaus-Gaddum-type invariant associated with the second Zagreb index is defined as follows $\widetilde{M}_2(G) = M_2(G) + M_2(\overline{G})$, where $\overline{G}$ is the complement of G, and let $\mathbb{G}_{n,m}$ be the family of all graphs with n vertices and m edges. Let $\mathbb{P}(G)$ be a parameter of G. A graph $G \in \mathbb{G}_{n,m}$ is said to be $\mathbb{P}$-maximal in $\mathbb{G}_{n,m}$ if

$$\mathbb{P}(G) = \max\{\mathbb{P}(H) : H \in \mathbb{G}_{n,m}\}.$$

Using an algebraic-combinatorial method, we in this paper show that, for any fixed (n, m), the extremal graphs in $\mathbb{G}_{n,m}$ maximizing M_1 and $\widetilde{M}_2$ coincide.

1 Introduction

Characterizing the graphs that attain the maximum or minimum value of a graph invariant over a fixed family of graphs is an important topic

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in extremal graph theory. The *first Zagreb index* $M_1(G)$ and *the second Zagreb index* $M_2(G)$ are two important graph invariants, defined as follows. Let G be a simple graph with degree sequence $(d_1, d_2, \ldots, d_n)$. For $i \in V(G)$, by $d_i = d_i(G)$ we denote the degree of the vertex i. Then

$$M_1(G) = \sum_{i=1}^{n} d_i^2, \qquad M_2(G) = \sum_{v_i v_j \in E(G)} d_i d_j.$$

These two Zagreb indices were introduced in the 1970s [11, 12]; historical accounts can be found in [9, 10, 18]. Originally devised to describe the extent of branching in the carbon-atom skeleton of molecules, they can be regarded as classical molecular structure-descriptors [4].

These two graph invariants are closely related to numerous graph-theoretic parameters. In 1978, Ahlswede and Katona [2] found that, for any given graph G, the number of pairs of different edges that have a common vertex–or equivalently, the number of edges in its line graph–equals its first Zagreb index $M_1(G)$. Oliveira et al. later derived an identity connecting the third Laplacian coefficient of a graph with its first Zagreb index $M_1(G)$; see [8, Theorem 3.1]. Recently, the first author et al. [14] established the following algebraic connection:

$$W_2(G) = \|A^2\| = M_1(G), \qquad W_3(G) = \|A^3\| = 2M_2(G),$$

where $W_\ell(G)$ denotes the number of walks with length ℓ and A is the adjacency matrix of G and $\|\cdot\|$ denotes the sum of all entries. In fact, the relationship $\|A^2\| = M_1(G)$ can be dated back to the work of Katz [15].

Denote by $\mathbb{G}_{n,m}$ the family of all graphs with n vertices and m edges. Let $\mathbb{P}(G)$ be a parameter of G. A graph $G \in \mathbb{G}_{n,m}$ is said to be $\mathbb{P}$-maximal in $\mathbb{G}_{n,m}$ if

$$\mathbb{P}(G) = \max\{\mathbb{P}(H) : H \in \mathbb{G}_{n,m}\}.$$

A graph is called *threshold* if it contains no $2P_2$, C_4, or P_4 as an induced subgraph [7, 17]. M_1-maximal graphs and M_2-maximal graphs are all threshold graphs.

The problem of characterizing the M_1-maximal graphs within $\mathbb{G}_{n,m}$ has a long history. Dating back to the work of Katz et al. [15] in 1971, subsequent contributions were made by Ahlswede and Katona [2], Peled, Petreschi and Sterbini [20], and Byer [6]; the problem was ultimately resolved by Ábrego et al. in 2009; see [1, Theorems 2.5-2.8], marking a research span of nearly forty years for M_1-maximal graphs within $\mathbb{G}_{n,m}$. In 1999, Bollobás et al. [5] showed that each graph with M_2-maximal graphs within $\mathbb{G}_{n,m}$ is threshold. In 2024, the first author et al. confirmed the conjecture proposed by Xu et al. [22] concerning the graph achieving the maximum value of $M_2(G)$ within $\mathbb{G}_{n,m}$; see [13, Theorem 1.1].

For a graph G, the chromatic number $\chi(G)$ is the minimum number of colors needed to color the vertices of G in such a way that no two adjacent vertices are assigned the same color. The complement of a graph G, denoted by $\overline{G}$, is the graph with the same vertex set as G, where two vertices are adjacent if and only if they are not adjacent in G. In 1956, Nordhaus and Gaddum [19] gave the bounds involving the chromatic number $\chi(G)$ of a graph G and its complement. Since then, for a given graph parameter $\mathbb{P}(G)$, problems concerning bounds on combinations of the form $\mathbb{P}(G)$ and $\mathbb{P}(\overline{G})$ –in particular their sums and products – have been referred to as Nordhaus–Gaddum problems [3]. Motivated by this tradition, we consider the following Nordhaus–Gaddum variant for the second Zagreb index. Especially, set

$$\widetilde{M_2}(G) = M_2(G) + M_2(\overline{G}).$$

For more information concerning Nordhaus-Gaddum-type variants, we refer the reader to the survey [3].

In this paper, we further elaborate on the close relationship between those two Zagreb indices and reveal the following interesting phenomenon.

Theorem 1. *For any integers n and m, the M_1-maximal graphs and the $\widetilde{M_2}$-maximal graphs coincide over the graph class $\mathbb{G}_{n,m}$.*

The rest of the paper is organized as follows. In section 2, we give some preliminaries. Then, in section 3, we complete the proof of Theorem 1.

2 Preliminaries

In this section, we will introduce the notations and terminologies, which will be utilized in the subsequent discussion.

Let G be a threshold graph with vertex set $\{v_1, v_2, \ldots, v_n\}$ such that

$$d_1 \geq d_2 \geq \cdots \geq d_n,$$

where d_i denotes the degree of the vertex v_i. The adjacency matrix of G whose the i-th row corresponds to the vertex d_i is said to be *the Ferrers matrix* of G. That is, for a threshold graph, its Ferrers matrix refers to the adjacency matrix with all ones maximally concentrated in the upper-left region. Ferrers matrix is also named as Ferrers diagram [17] or stepwise matrix [21].

Let G be a threshold graph with Ferrers matrix F. The number of ones in the upper triangular part (or lower triangular part) of F on each of the anti-diagonal lines is called *the diagonal sequence* of G, denoted by $\delta(G)$. For example, the diagonal sequences of the threshold graph G_1 and G_2 depicted in Figure 1 are both $\delta(G) = (1, 1, 2, 2, 3, 3, 3, 1, 1)$, where entries 1 are represented by solid circles, while entries 0 are denoted by hollow circles. This example demonstrates that a threshold graph is not uniquely determined by its diagonal sequence.

Let $F = (f_{ij})$ be the Ferrers diagram of the threshold graph G. The entry (i, j) is called an *outer-corner* of the Ferrers diagram F if $f_{ij} = 1$ and $f_{i,j+1} = f_{i+1,j} = 0$. The entry (p, q) is called an *inner-corner* of F if $f_{p-1,q} = f_{p,q-1} = 1$ and $f_{p,q} = 0$. Obviously, the graph $G + pq$ (resp. $G - pq$) is also a threshold graph if and only if (p, q) is an inner-corner (resp. an outer-corner) of G.

3 Proof of Theorem 1

In this section, we will complete the proof of Theorem 1 by establishing two equivalent theorems.

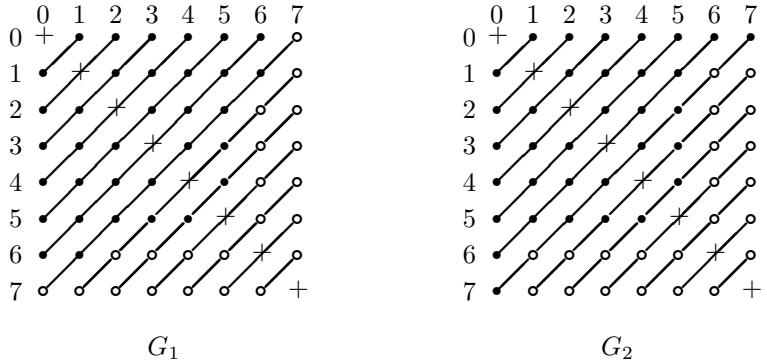

Figure 1. Distinct threshold graphs having the same diagonal sequence $(1, 1, 2, 2, 3, 3, 3, 1, 1)$.

We start with the following lemma from [13], which settles the conjecture on the characterization of M_2-maximal graphs. We include its proof here for completeness. We emphasize that, for convenience, the rows and columns of the Ferrers matrix in this paper are indexed starting from 0.

Lemma 1 ([13], Lemma 2.1)**.** *Let F be the Ferrers matrix of a threshold graph G within $\mathbb{G}_{n,m}$. If (i, j) with $1 \leq j < i \leq n-1$ is an inner-corner of F, then*

$$M_2(G + ij) - M_2(G) = 2m + 2ij - j + 1.$$

Proof. Applying the property of threshold graphs, $d_i(G) = j$, $d_j(G) = i-1$, $N_i(G+ij) = \{0, 1, \ldots, j\}$ and $N_j(G+ij) = \{0, 1, \ldots, j-1, j+1, \ldots, i\}$. Thus $d_i(G + ij) = j + 1$ and $d_j(G + ij) = i$. Consequently, we have

$$\begin{aligned} M_2(G + ij) - M_2(G) &= \sum_{s=0, s\neq j}^{i-1} d_s(G) + \sum_{t=0}^{j-1} d_t(G) + d_i(G + ij)d_j(G + ij) \\ &= \left(\sum_{s=0}^{i-1} d_s(G) - d_j(G) \right) + \sum_{t=0}^{j-1} d_t(G) + (j + 1)i \\ &= (2m - j) + (i - 1)j + (j + 1)i \\ &= 2m + 2ij - j + 1. \end{aligned}$$

■

Applying Lemma 1, we have

Lemma 2. *Let $G \in \mathbb{G}_{n,m}$ be a threshold graph with Ferrers matrix F. If (i,j) with $1 \leq j < i \leq n-1$ is an inner-corner of F, then*

$$\widetilde{M}_2(G+ij) - \widetilde{M}_2(G) = 4m - 3n^2 + 6n - 1 + (2n-3)(i+j).$$

Proof. Denote by $\overline{F}$ the Ferrers matrix of the graph $\overline{G}$. By the definition of a Ferrers matrix, we have $\overline{F} = D^T(J - I - F)D$, where D is the anti-diagonal matrix satisfy $d_{i,n-i} = 1$ for $i = 0, \ldots, n-1$ and $d_{i,j} = 0$ otherwise, J is the all ones square matrix and I is the identity matrix. In view of (i,j) is an inner-corner of F, then (p,q) is an outer-corner of $\overline{F}$, where $p = n-j-1$ and $q = n-i-1$. Therefore, $\overline{G+ij} = \overline{G} - pq$. Consequently, we have

$$\begin{aligned}
\widetilde{M}_2(G+ij) - \widetilde{M}_2(G) &= M_2(G+ij) + M_2(\overline{G+pq}) - (M_2(G) + M_2(\overline{G})) \\
&= 2m + 2ij - j + 1 - n(n-1) + 2m - 2pq + p - 1 \\
&= 4m + 2ij - j - 2pq + p - n(n-1) \\
&= 4m + 2ij - j - 2(n-j-1)(n-i-1) \\
&\quad + (n-j-1) - n(n-1) \\
&= 4m - 3n^2 + 6n - 1 + (2n-3)(i+j).
\end{aligned}$$

Then the proof is complete. ∎

As a consequence of Lemma 2, we have

Theorem 2. *Let $G \in \mathbb{G}_{n,m}$ be a threshold graph with Ferrers matrix F. Then*

$$\widetilde{M}_2(G) = \frac{n(n-1)^3}{2} + 2m(m-1) - m(3n^2 - 6n + 1) + \frac{(2n-3)}{2} \sum_{f_{ij}=1} (i+j),$$

where the sum runs over all 1-entries.

Proof. Let $(G_0, G_1, \ldots, G_m = G)$ be an arbitrary threshold graph sequence such that $G_k \in \mathbb{G}_{n,k}$ for $k = 0, 1, \ldots, m$ and G_k is the graph obtained from G_{k-1} by adding an edge. For each k, denote by F_k is the Ferrers

matrix of the threshold graph G_k. Then $G_0 = \overline{K}_n$ and thus $\widetilde{M}_2(G_0) = M_2(\overline{K}_n) + M_2(K_n) = \frac{n(n-1)^3}{2}$. Furthermore, by the construction of above threshold graph sequence, F_k is the matrix obtained from F_{k-1} by changing some inner-corner entry (i_{k-1}, j_{k-1}) together with its symmetric entry (j_{k-1}, i_{k-1}) from 0 to 1. Note that we only consider the entries in the upper-triangular(or lower-triangular) when relating edge sums to matrix sums. Therefore, by Lemma 2, we have

$$\widetilde{M}_2(G_k) - \widetilde{M}_2(G_{k-1}) = 4(k-1) - 3n^2 + 6n - 1 + (2n-3)(i_{k-1} + j_{k-1})$$

for $k = 1, \ldots, m$. Summing over k,

$$\begin{aligned}
&\widetilde{M}_2(G) - \widetilde{M}_2(G_0) \\
&= \sum_{k=1}^{m} \big[4(k-1) - 3n^2 + 6n - 1\big] + (2n-3) \sum_{k=1}^{m} (i_{k-1} + j_{k-1}) \\
&= \sum_{k=1}^{m} \big[4(k-1) - 3n^2 + 6n - 1\big] + \frac{2n-3}{2} \sum_{f_{ij}=1} (i+j) \\
&= 2m(m-1) - m(3n^2 - 6n + 1) + \frac{2n-3}{2} \sum_{f_{ij}=1} (i+j),
\end{aligned}$$

the second equation holds because each 1-entry of $F_m (= F(G))$ is an inner-corner of some Ferrers matrix in the sequence $(F_0, F_1, \ldots, F_{m-1})$. Therefore, the proof is complete. ■

From Theorem 2, we can partition $\widetilde{M}_2(G)$ into two parts: $\frac{n(n-1)^3}{2} + 2m(m-1) - m(3n^2 - 6n + 1)$ and $\frac{(2n-3)}{2} \sum_{f_{ij}=1} (i+j)$. The former is a constant, determined jointly by the number of vertices and edges contained in G. The latter is determined jointly by the number of vertices of G and the positions of those edges.

Due to Ábrego et al., a representation of $M_1(G)$ in terms of its diagonal sequence is given.

Lemma 3 ([1], Lemma 2)**.** *Let G be a threshold graph with diagonal*

sequence $\delta(G) = (\delta_1, \delta_2, \ldots, \delta_t)$. *Then*

$$M_1(G) = 2\delta(G) \cdot (1, 2, 3, \ldots, t) = 2\sum_{i=1}^{t} i\delta_i.$$

Applying Lemma 3, we provide an alternative representation of $M_1(G)$ of a threshold graph G in terms of its Ferrers matrix.

Theorem 3. *Let G be a threshold graph with Ferrers matrix $F = [f_{ij}]_{n\times n}$. Then*

$$M_1(G) = \sum_{f_{ij}=1} (i + j),$$

where the sum runs over all entries 1.

Proof. First, we observe that the sum of the x- and y-coordinates of each entry equal to 1 coincides with the order of its corresponding diagonal in the diagonal sequence. We emphasize once again that the rows and columns of a Ferrers matrix are indexed starting from 0. Consequently, each term $i\delta_i$ in Lemma 3 can be interpreted as the sum of the x- and y-coordinates of the $2\delta_i$ entries lying on the i-th anti-diagonal. Therefore, the result then follows immediately. ■

Putting Theorem 2 into Theorem 3, we have

Corollary. *Let $G \in \mathbb{G}_{n,m}$ be a threshold graph with diagonal sequence $\delta(G) = (\delta_1, \delta_2, \ldots, \delta_t)$. Then*

$$\widetilde{M_2}(G) = \frac{n(n-1)^3}{2} + 2m(m-1) - m(3n^2 - 6n + 1) + \frac{(2n-3)}{2}\sum_{k=1}^{t} k\delta_k.$$

Motivated by Theorems 2 and 3, we give the following definition.

Definition 1. Let $G, H \in \mathbb{G}_{n,m}$ be two threshold graphs with diagonal sequences $\delta(G) = (\delta_1, \ldots, \delta_s)$ and $\delta(H) = (\delta'_1, \ldots, \delta'_t)$, respectively. We say that $\delta(G)$ is *no less* than $\delta(H)$, denoted by $\delta(G) \succeq \delta(H)$, if $s \geq t$ and

$$\sum_{i=1}^{k} (\delta_i - \delta'_i)$$

is non-positive for all $k = 1, 2, \ldots, s$. Furthermore, $\delta(G)$ is *greater* than $\delta(H)$, written as $\delta(G) \succ \delta(H)$, if $\delta(G) \succeq \delta(H)$ and $\sum_{i=1}^{k}(\delta_i - \delta'_i)$ is negative for at least one index $k \in \{1, 2, \ldots, t\}$.

Definition 2. Let $G \in \mathbb{G}_{n,m}$ be a threshold graph with diagonal sequence $\delta(G) = (\delta_1, \ldots, \delta_s)$. We say that $\delta(G)$ is *greatest* if $\delta(G)$ is no less than any diagonal sequence of H contained in $\mathbb{G}_{n,m}$.

Example. Both graphs G_1 and G_2 illustrated in Figure 1 belong to $\mathbb{G}_{8,17}$. One can verify that $\delta(G_1) = \delta(G_2)$, and their diagonal sequences are not less than that of any other threshold graph in $\mathbb{G}_{8,17}$ except G_1 and G_2 themselves. Specifically, $\delta(G_1) = \delta(G_2) \succ (1, 1, 2, 2, 3, 3, 3, 2)$, where $(1, 1, 2, 2, 3, 3, 3, 2)$ is the diagonal sequence of the quasi-star graph $S_{8,17}$. Thus both $\delta(G_1)$ and $\delta(G_2)$ are greatest diagonal sequence among all graphs in $\mathbb{G}_{8,17}$.

As a consequence of Theorem 2, we give a characterization on the $\widetilde{M}_2$-maximal graphs in $\mathbb{G}_{n,m}$ as follows.

Theorem 4. *Let $G \in \mathbb{G}_{n,m}$ be a threshold graph with diagonal sequences $\delta(G)$. Then G is $\widetilde{M}_2$-maximal if and only if $\delta(G)$ is greatest among all diagonal sequences of threshold graphs contained in $\mathbb{G}_{n,m}$.*

Proof. It suffices to prove that $\widetilde{M}_2(G) > \widetilde{M}_2(H)$ if $\delta(G) \succneqq \delta(H)$, where $G, H \in \mathbb{G}_{n,m}$. Let $\delta(G) = (\delta_1, \ldots, \delta_s)$ and $\delta(H) = (\delta'_1, \ldots, \delta'_t)$ with $s \geq t$(set $\delta'_k = 0$ for $k > t$). Then by Corollary 3

$$\widetilde{M}_2(G) - \widetilde{M}_2(H) = \frac{2n-3}{2} \sum_{k=1}^{s} k(\delta_k - \delta'_k). \tag{3.1}$$

In view of $G, H \in \mathbb{G}_{n,m}$, then

$$\sum_{i=1}^{s} \delta_i = \sum_{i=1}^{t} \delta'_i = m.$$

Since $\delta(G) \succneqq \delta(H)$, by Definition 1 each positive unit entry corresponds to a positive unit entry whose index is smaller, then $\widetilde{M}_2(G) - \widetilde{M}_2(H) > 0$ and thus the result follows. ∎

Remark. Similar to Lemma 1 or Lemma 2, we can show that

$$M_1(G+ij) - M_1(G) = 2(i+j),$$

where $G \in G_{n,m}$ and (i,j) is an inner-corner of the Ferrers matrix associated to G. Theorem 3 can then be established by an analogous argument to that used for Theorem 4.

Consequently, we give another characterization on the M_1-maximal graphs in $\mathbb{G}_{n,m}$.

Theorem 5. *Let $G \in \mathbb{G}_{n,m}$ be a threshold graph with diagonal sequences $\delta(G)$. Then G is M_1-maximal if and only if $\delta(G)$ is greatest among all diagonal sequences contained in $\mathbb{G}_{n,m}$.*

Proof. Let $\delta(G) = (\delta_1, \ldots, \delta_s)$ and $\delta(H) = (\delta'_1, \ldots, \delta'_t)$ with $s \geq t$(set $\delta'_i = 0$ for $i > t$). Combining Lemma 3 and the method of Theorem 3, we have

$$M_1(G) - M_1(H) = 2\sum_{i=1}^{s} i(\delta_i - \delta'_i) > 0.$$

Then the result follows. ■

Proof of Theorem 1. Putting Theorem 4 into Theorem 5, the result follows.

Remark. Different graphs may have identical diagonal sequences, or even identical greatest diagonal sequences. This explains why an M_1-maximal graph, as well as $\widetilde{M}_2$-maximal graph, need not be unique; see Theorems 2.3-2.8 in [1] for details.

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